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Thermodynamic functions of lactones in the gaseous state

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Abstract

© 2016, Springer Science+Business Media New York.The temperature dependences of the vapor pressures of oxacyclobutan-2-one and oxacyclopentan-2-one were measured by the transpiration method. The entropies of gaseous oxacycloalkan-2-ones (lactones) were determined based on the experimental values of entropy in the condensed state, vapor pressure, and enthalpy of vaporization. Thermodynamic functions of lactones with a ring size of n = 4—8 (number of atoms in the ring) were determined by quantum chemistry and statistical physics methods in the ideal gas approximation taking into account the molar fractions of all conformers and optical isomers in the temperature range from 298.15 to 1500 K. The enthalpies of ring strain were calculated based on the enthalpies of formation.

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Keywords

anharmonic frequencies, enthalpy of formation, enthalpy of ring strain, entropy, free energy, heat capacity, lactone, rigid rotor—anharmonic oscillator